Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 09:14 AM EST

PDB ID	:	6BOG
Title	:	Crystal structure of RapA, a Swi2/Snf2 protein that recycles RNA polymerase during transcription
Authors	:	Shaw, G.X.; Gan, J.; Zhou, Y.N.; Zhang, R.; Joachimiak, A.; Jin, D.J.; Ji, X.
Deposited on	:	2017-11-20
Resolution	:	3.21 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

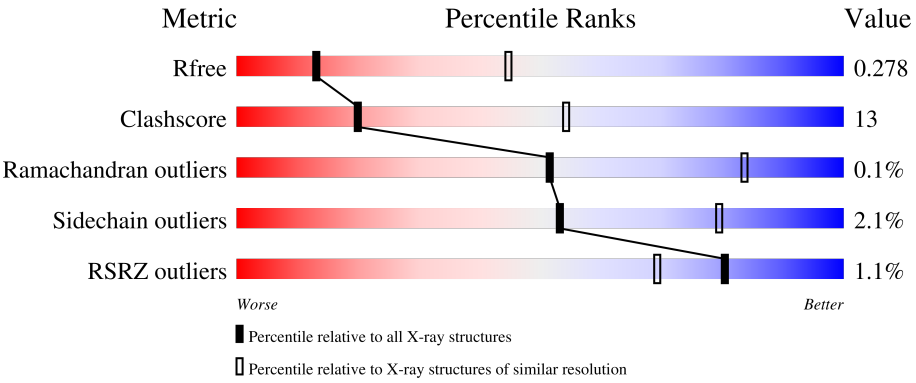
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

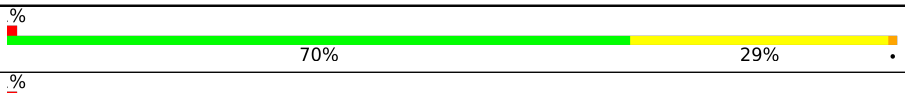
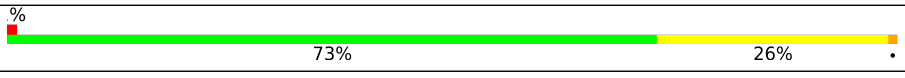
The reported resolution of this entry is 3.21 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	968	
1	B	968	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	1003	-	-	X	-
2	SO4	B	1002	-	-	X	-
2	SO4	B	1003	-	-	X	-

2 Entry composition

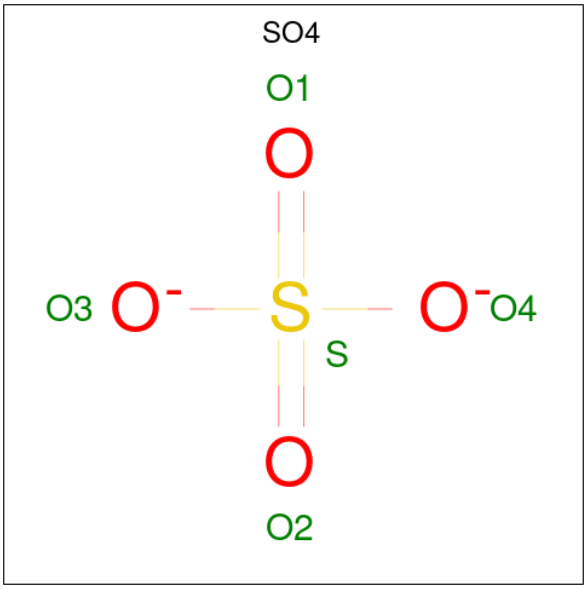
There are 2 unique types of molecules in this entry. The entry contains 15473 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RNA polymerase-associated protein RapA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	967	Total	C	N	O	S	Se	0	0	0
			7719	4831	1382	1477	6	23			
1	B	967	Total	C	N	O	S	Se	0	0	0
			7719	4831	1382	1477	6	23			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	O	S		0	0
			5	4	1			
2	A	1	Total	O	S		0	0
			5	4	1			
2	A	1	Total	O	S		0	0
			5	4	1			
2	B	1	Total	O	S		0	0
			5	4	1			

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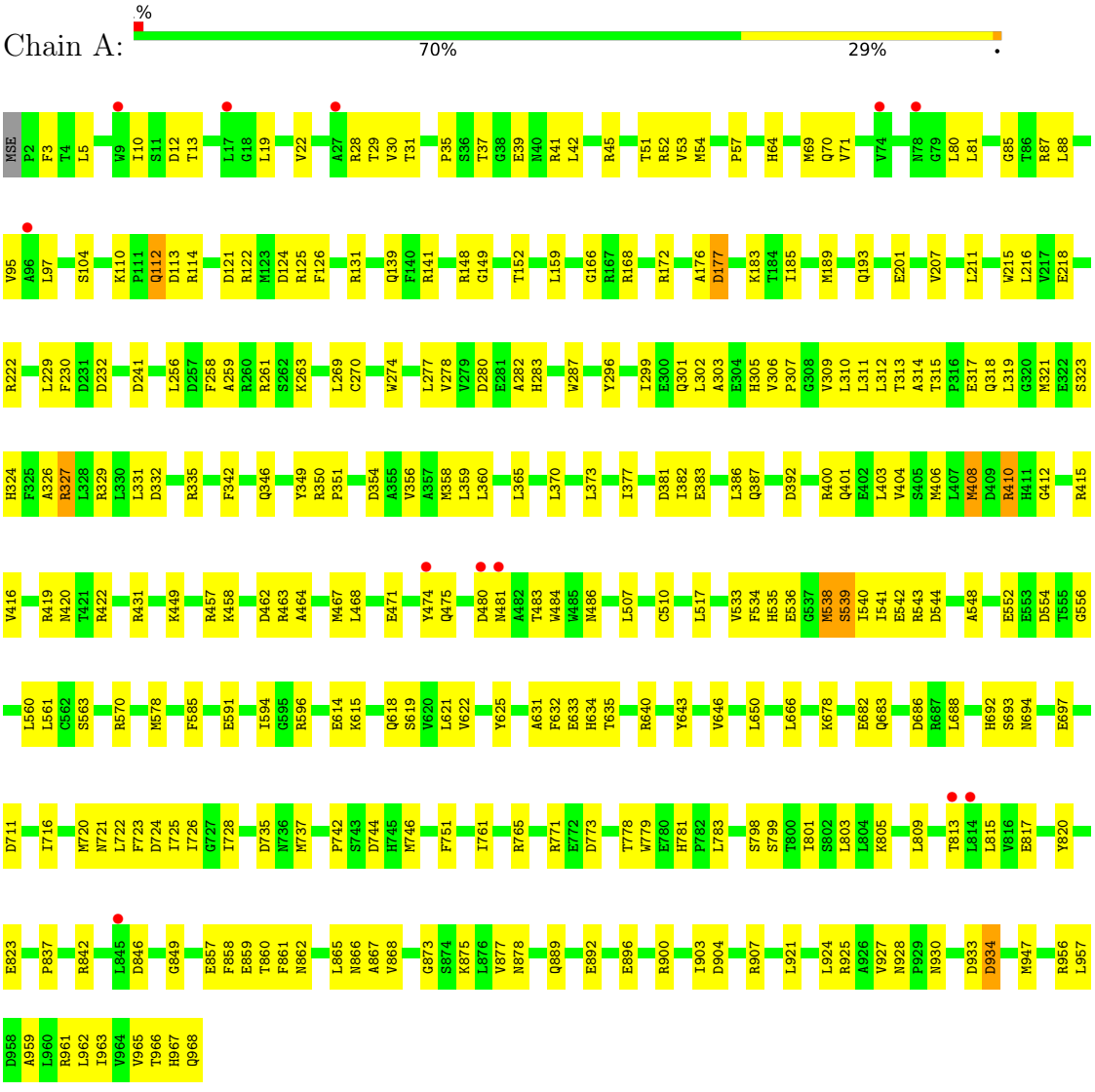
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

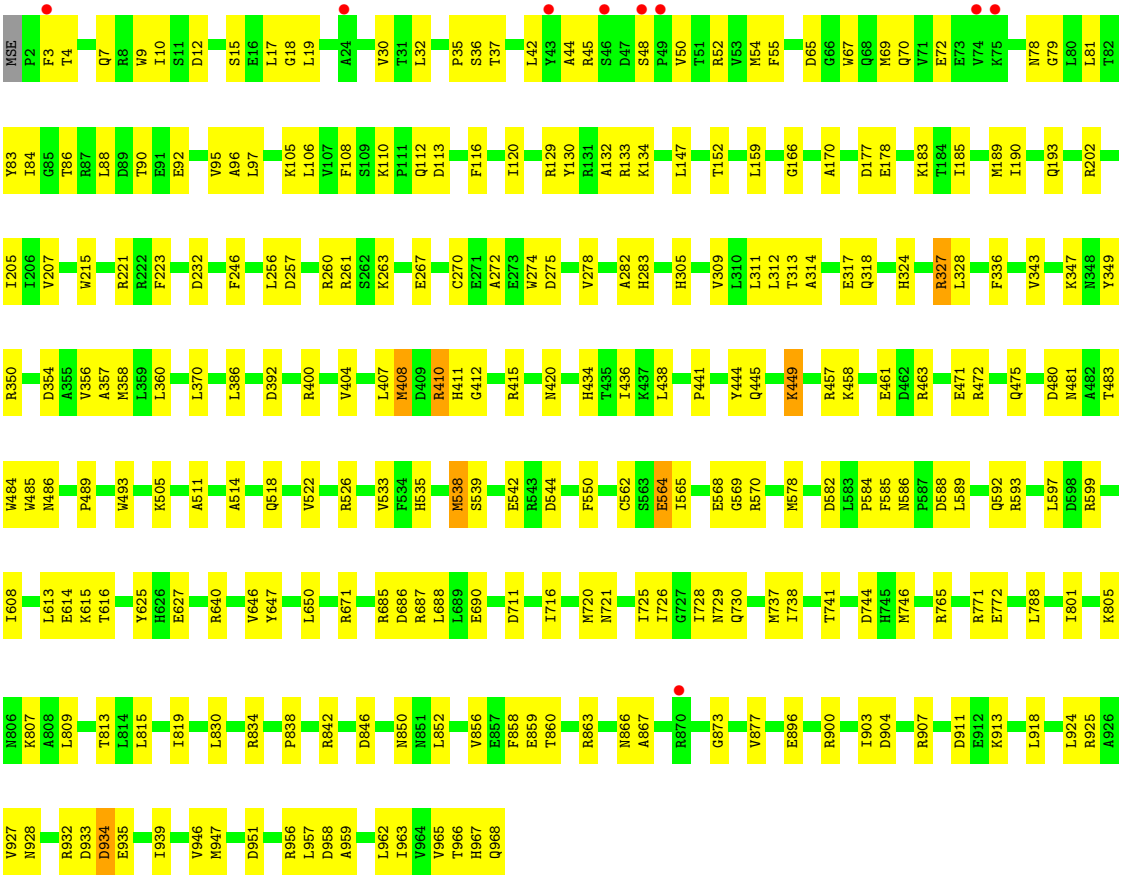
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: RNA polymerase-associated protein RapA



• Molecule 1: RNA polymerase-associated protein RapA


MSE P2 F3 T4 Q7 R8 W9 I10 S11 D12 S15 E16 L17 G18 L19 A24 V30 T31 L32 P35 S36 T37 L42 Y43 A44 R45 S46 D47 S48 P49 V50 T51 R52 V53 M54 F55 D65 G66 W67 Q68 M69 Q70 V71 E72 E73 V74 K75 N78 G79 L80 L81 T82
Y83 I84 G85 T86 R87 L88 D89 T90 E91 E92 V95 A96 L97 K105 L106 V107 F108 S109 K110 P111 Q112 D113 F116 I120 R129 Y130 R131 A132 R133 K134 L147 T152 L159 G166 A170 D177 E178 K183 T184 I185 M189 I190 Q193 R202
I205 I206 V207 W215 R221 R222 F223 D232 F246 L256 D257 R260 R261 S262 K263 E267 C270 E271 A272 E273 W274 D275 V278 A282 H283 H305 V309 L310 L311 L312 T313 A314 E317 Q318 H324 R327 L328 F336 V343 K347 N348 Y349
R350 D354 A355 V356 A357 M358 L359 L360 L370 L386 D392 R400 V404 L407 M408 D409 R410 H411 G412 R415 N420 H434 T435 I436 K437 L438 P441 Y444 Q445 K449 R457 K458 E461 D462 R463 E471 R472 Q475 D480 N481 A482 T483
W484 W485 N486 P489 W493 K505 A511 A514 Q518 V522 R526 V533 F534 H535 M538 S539 E542 R543 D544 F550 C562 S563 E564 I565 E568 G569 R570 M578 D582 L583 P584 F585 N586 P587 D588 L589 Q592 R593 L597 D598 R599
I608 L613 E614 K615 T616 Y625 H626 E627 R640 V646 Y647 L650 R671 R685 D686 R687 L688 L689 E690 D711 I716 M720 N721 I725 I726 G727 I728 N729 Q730 M737 I738 T741 D744 H745 M746 R765 R771 E772 L788 I801 K805
N806 K807 A808 L809 T813 L814 L815 I819 L830 R834 P838 R842 D846 N850 N851 L852 V856 E857 F858 E859 T860 R863 N866 A867 R870 G873 V877 E896 R900 I903 D904 R907 D911 E912 K913 L918 L924 R925 A926
V927 N928 R932 D933 D934 E935 I939 V946 M947 D951 R956 L957 D958 A959 L962 I963 V964 V965 T966 H967 Q968

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	123.86Å 123.86Å 187.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.19 – 3.21 29.19 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.19-3.21) 98.9 (29.19-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 3.18Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.244 , 0.279 0.245 , 0.278	Depositor DCC
R_{free} test set	994 reflections (2.17%)	wwPDB-VP
Wilson B-factor (Å^2)	91.6	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 38.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.449 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for h,-k,-l	Depositor
Outliers	0 of 45884 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	15473	wwPDB-VP
Average B, all atoms (Å^2)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.31	0/7840	0.53	0/10581
1	B	0.29	0/7840	0.53	0/10581
All	All	0.30	0/15680	0.53	0/21162

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7719	0	7583	208	0
1	B	7719	0	7583	183	0
2	A	15	0	0	3	0
2	B	20	0	0	5	0
All	All	15473	0	15166	386	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (386) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:VAL:O	1:B:538:MSE:HE1	1.35	1.22
1:B:737:MSE:HE1	1:B:771:ARG:NH1	1.90	0.85
1:A:540:ILE:HD13	1:A:543:ARG:NH2	1.95	0.81
1:B:70:GLN:HB3	1:B:86:THR:HB	1.62	0.80
1:A:540:ILE:CD1	1:A:543:ARG:NH2	2.47	0.77
1:B:67:TRP:HH2	1:B:97:LEU:HD11	1.51	0.74
1:B:7:GLN:NE2	1:B:79:GLY:O	2.20	0.73
1:B:317:GLU:O	1:B:318:GLN:HG2	1.89	0.72
1:A:64:HIS:O	1:B:925:ARG:NH1	2.23	0.72
1:B:627:GLU:O	1:B:671:ARG:NH1	2.23	0.71
1:A:280:ASP:HA	1:A:312:LEU:HB2	1.72	0.71
1:A:536:GLU:O	1:A:536:GLU:HG2	1.89	0.71
1:A:483:THR:OG1	1:A:486:ASN:ND2	2.23	0.71
1:A:114:ARG:NH1	1:A:799:SER:OG	2.24	0.70
1:A:809:LEU:O	1:A:967:HIS:NE2	2.21	0.70
1:B:70:GLN:HB2	1:B:88:LEU:HD21	1.72	0.70
1:A:168:ARG:NH2	1:A:415:ARG:O	2.23	0.70
1:A:110:LYS:HB3	1:A:112:GLN:OE1	1.92	0.69
1:A:166:GLY:HA3	1:A:193:GLN:NE2	2.07	0.69
1:A:538:MSE:HE3	1:A:542:GLU:HB3	1.75	0.69
1:A:925:ARG:NH2	1:A:933:ASP:OD1	2.21	0.69
1:A:172:ARG:HB3	1:A:331:LEU:HD22	1.74	0.68
1:A:722:LEU:HD11	1:A:726:ILE:HD11	1.76	0.68
1:A:817:GLU:OE2	1:A:961:ARG:NH2	2.27	0.68
1:A:131:ARG:NH1	1:A:859:GLU:OE1	2.27	0.68
1:A:646:VAL:HG12	1:A:650:LEU:HB2	1.76	0.67
1:B:410:ARG:HG3	1:B:927:VAL:HG13	1.76	0.67
1:B:221:ARG:HH12	1:B:570:ARG:HH12	1.41	0.67
1:A:324:HIS:HA	1:A:327:ARG:HH11	1.60	0.67
1:B:728:ILE:HG12	1:B:746:MSE:HE1	1.75	0.67
1:B:564:GLU:OE2	1:B:593:ARG:NH2	2.29	0.66
1:A:544:ASP:OD1	1:A:570:ARG:NH1	2.21	0.66
1:A:350:ARG:NH2	1:A:683:GLN:O	2.29	0.66
1:B:511:ALA:N	1:B:582:ASP:OD2	2.29	0.65
1:A:317:GLU:O	1:A:318:GLN:HG2	1.96	0.65
1:A:232:ASP:OD2	1:A:261:ARG:NH1	2.29	0.65
1:B:343:VAL:HG12	1:B:347:LYS:HE2	1.79	0.65
1:A:70:GLN:HB2	1:A:88:LEU:HD21	1.79	0.64
1:A:335:ARG:NE	1:A:930:ASN:OD1	2.28	0.64
1:B:70:GLN:N	1:B:86:THR:O	2.25	0.64
1:B:112:GLN:O	1:B:116:PHE:N	2.25	0.64
1:B:544:ASP:OD1	1:B:570:ARG:NH1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:588:ASP:OD2	1:B:640:ARG:NE	2.30	0.64
1:B:221:ARG:NH2	1:B:544:ASP:OD2	2.30	0.64
1:A:862:ASN:OD1	1:A:961:ARG:NH1	2.31	0.64
1:B:67:TRP:CH2	1:B:97:LEU:HD11	2.32	0.64
1:A:309:VAL:HG12	1:A:311:LEU:HD13	1.79	0.63
1:A:803:LEU:HD23	1:A:868:VAL:HG12	1.80	0.63
1:A:924:LEU:O	1:A:928:ASN:N	2.32	0.62
1:B:438:LEU:HD13	1:B:489:PRO:HB2	1.81	0.62
1:B:578:MSE:HE3	1:B:597:LEU:HD22	1.80	0.62
1:B:834:ARG:HH21	1:B:913:LYS:NZ	1.97	0.62
1:B:842:ARG:NH1	1:B:858:PHE:HD1	1.98	0.62
1:B:564:GLU:OE2	1:B:593:ARG:NE	2.31	0.61
1:B:584:PRO:HD3	1:B:593:ARG:NH1	2.16	0.61
1:B:685:ARG:HD2	1:B:690:GLU:OE2	2.00	0.61
1:B:813:THR:HG22	1:B:965:VAL:HB	1.83	0.61
1:B:309:VAL:HG12	1:B:311:LEU:HD13	1.82	0.61
1:B:484:TRP:NE1	1:B:518:GLN:OE1	2.31	0.61
1:B:614:GLU:HG2	1:B:615:LYS:HG2	1.82	0.61
1:B:232:ASP:OD1	1:B:261:ARG:NH2	2.34	0.60
1:A:359:LEU:HD21	1:A:400:ARG:HG2	1.82	0.60
1:A:621:LEU:HB3	1:A:625:TYR:CE2	2.36	0.60
1:B:48:SER:HB2	1:B:50:VAL:HG22	1.83	0.60
1:A:646:VAL:HG11	1:A:666:LEU:HD21	1.82	0.60
1:A:323:SER:O	1:A:327:ARG:NH1	2.35	0.60
1:B:129:ARG:NH2	1:B:958:ASP:OD1	2.24	0.60
1:A:35:PRO:HB2	1:A:104:SER:OG	2.02	0.60
1:B:282:ALA:HB3	1:B:313:THR:HB	1.83	0.59
1:B:183:LYS:N	2:B:1001:SO4:O2	2.34	0.59
1:A:538:MSE:HE3	1:A:542:GLU:CB	2.33	0.59
1:B:183:LYS:HB3	1:B:312:LEU:HD23	1.83	0.59
1:A:309:VAL:HG12	1:A:311:LEU:CD1	2.31	0.59
1:A:813:THR:HG22	1:A:965:VAL:HB	1.84	0.59
1:A:966:THR:OG1	1:A:968:GLN:OE1	2.21	0.59
1:B:328:LEU:HB3	1:B:336:PHE:CE2	2.38	0.59
1:A:87:ARG:HB2	1:A:95:VAL:HG21	1.86	0.58
1:A:857:GLU:OE2	1:A:860:THR:HG23	2.04	0.58
1:A:815:LEU:HB2	1:A:963:ILE:HB	1.86	0.58
1:A:823:GLU:OE2	1:A:956:ARG:NH2	2.36	0.58
1:B:270:CYS:HB3	1:B:305:HIS:CG	2.38	0.58
1:A:277:LEU:O	1:A:310:LEU:N	2.33	0.58
1:B:3:PHE:CD2	1:B:45:ARG:HG2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ILE:HG21	1:B:801:ILE:HG22	1.84	0.57
1:A:471:GLU:O	1:A:475:GLN:HG3	2.04	0.57
1:A:517:LEU:HD22	1:A:533:VAL:HG11	1.85	0.57
1:A:185:ILE:HG22	1:A:189:MSE:SE	2.54	0.57
1:B:472:ARG:NH1	1:B:514:ALA:HB3	2.19	0.57
1:B:445:GLN:HB3	1:B:449:LYS:HZ1	1.69	0.57
1:A:110:LYS:NZ	1:A:112:GLN:OE1	2.37	0.57
1:A:335:ARG:NH2	1:A:412:GLY:O	2.38	0.57
1:A:349:TYR:HE1	1:A:688:LEU:HD12	1.70	0.56
1:B:471:GLU:O	1:B:475:GLN:HG3	2.05	0.56
1:A:85:GLY:O	1:A:95:VAL:N	2.38	0.56
1:B:10:ILE:HB	1:B:15:SER:OG	2.04	0.56
1:B:257:ASP:OD1	1:B:260:ARG:NH1	2.31	0.56
1:B:83:TYR:O	1:B:97:LEU:N	2.30	0.56
1:A:422:ARG:NE	1:A:635:THR:HG21	2.19	0.56
1:A:354:ASP:O	1:A:358:MSE:HG2	2.06	0.56
1:A:858:PHE:N	2:A:1003:SO4:O3	2.32	0.56
1:B:415:ARG:HH22	1:B:935:GLU:CD	2.09	0.56
1:B:166:GLY:HA3	1:B:193:GLN:NE2	2.21	0.56
1:B:178:GLU:HB2	1:B:420:ASN:O	2.06	0.55
1:B:925:ARG:NH2	1:B:933:ASP:OD1	2.39	0.55
1:A:431:ARG:NH2	1:A:631:ALA:O	2.40	0.55
1:A:176:ALA:O	1:A:419:ARG:NH1	2.32	0.55
1:B:3:PHE:HD2	1:B:45:ARG:HG2	1.72	0.55
1:B:130:TYR:OH	2:B:1003:SO4:O3	2.25	0.55
1:A:415:ARG:HG2	1:A:415:ARG:HH11	1.71	0.55
1:A:801:ILE:HG13	1:A:962:LEU:HB2	1.89	0.55
1:B:918:LEU:HB2	1:B:939:ILE:HG21	1.89	0.54
1:A:842:ARG:NH1	1:A:858:PHE:HD1	2.06	0.54
1:A:358:MSE:HB2	1:A:365:LEU:HD21	1.90	0.54
1:A:3:PHE:HE2	1:A:45:ARG:HG2	1.72	0.54
1:A:539:SER:OG	1:A:542:GLU:HG3	2.07	0.54
1:A:728:ILE:HG12	1:A:746:MSE:HE1	1.88	0.54
1:B:10:ILE:HG21	1:B:106:LEU:HD11	1.90	0.54
1:B:911:ASP:HB2	1:B:947:MSE:HE2	1.89	0.54
1:A:614:GLU:HG2	1:A:615:LYS:HG2	1.90	0.54
1:B:349:TYR:OH	1:B:686:ASP:OD1	2.26	0.54
1:B:461:GLU:HG3	1:B:647:TYR:OH	2.07	0.54
1:A:19:LEU:HD21	1:A:53:VAL:HG11	1.89	0.54
1:A:857:GLU:HG2	2:A:1003:SO4:O3	2.08	0.53
1:B:538:MSE:HG2	1:B:542:GLU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ARG:NE	1:B:272:ALA:O	2.41	0.53
1:B:568:GLU:HA	1:B:599:ARG:NH2	2.22	0.53
1:B:485:TRP:HE1	1:B:526:ARG:NH2	2.06	0.53
1:B:873:GLY:O	1:B:877:VAL:HG23	2.08	0.53
1:A:324:HIS:HA	1:A:327:ARG:NH1	2.24	0.53
1:A:431:ARG:HB2	1:A:633:GLU:HA	1.91	0.53
1:B:807:LYS:HA	1:B:967:HIS:HD2	1.74	0.53
1:B:480:ASP:OD1	1:B:481:ASN:N	2.41	0.53
1:A:585:PHE:O	1:A:625:TYR:OH	2.26	0.53
1:A:370:LEU:HD13	1:A:386:LEU:HD21	1.91	0.52
1:A:771:ARG:NH2	1:A:773:ASP:OD2	2.23	0.52
1:A:907:ARG:HH21	1:A:947:MSE:HB3	1.72	0.52
1:A:535:HIS:O	1:A:538:MSE:HG3	2.09	0.52
1:B:415:ARG:HH11	1:B:415:ARG:HG2	1.74	0.52
1:A:907:ARG:HE	1:A:947:MSE:HG2	1.73	0.52
1:A:507:LEU:HD12	1:A:560:LEU:HB3	1.91	0.52
1:A:900:ARG:HH21	1:A:903:ILE:HG21	1.75	0.52
1:B:54:MSE:HG2	1:B:81:LEU:HD11	1.91	0.52
1:A:726:ILE:HG22	1:A:746:MSE:SE	2.60	0.51
1:A:751:PHE:HE2	1:A:783:LEU:HD22	1.75	0.51
1:B:445:GLN:HB3	1:B:449:LYS:NZ	2.24	0.51
1:B:900:ARG:HH21	1:B:903:ILE:HG12	1.75	0.51
1:A:480:ASP:OD1	1:A:481:ASN:N	2.43	0.51
1:A:172:ARG:HE	1:A:331:LEU:HA	1.76	0.51
1:B:415:ARG:NH2	1:B:935:GLU:OE1	2.43	0.51
1:A:10:ILE:HG23	1:A:53:VAL:HG21	1.92	0.51
1:A:172:ARG:O	1:A:416:VAL:HG23	2.11	0.51
1:B:147:LEU:HG	1:B:159:LEU:HD22	1.93	0.51
1:B:283:HIS:HB3	1:B:314:ALA:O	2.11	0.51
1:B:408:MSE:HG2	1:B:688:LEU:HD22	1.92	0.51
1:B:458:LYS:O	1:B:463:ARG:HD3	2.11	0.51
1:B:350:ARG:NH2	1:B:685:ARG:O	2.43	0.51
1:A:716:ILE:O	1:A:720:MSE:HG3	2.11	0.50
1:B:72:GLU:OE2	1:B:86:THR:OG1	2.20	0.50
1:B:133:ARG:HH12	1:B:838:PRO:HB2	1.76	0.50
1:B:538:MSE:HG2	1:B:542:GLU:CB	2.41	0.50
1:B:815:LEU:HB2	1:B:963:ILE:HB	1.93	0.50
1:A:383:GLU:O	1:A:387:GLN:HG2	2.12	0.50
1:A:552:GLU:HB2	1:A:556:GLY:HA3	1.93	0.50
1:A:110:LYS:HB3	1:A:110:LYS:HZ2	1.75	0.50
1:B:4:THR:HG21	1:B:78:ASN:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:CYS:O	1:A:563:SER:HA	2.11	0.50
1:B:805:LYS:HG2	1:B:966:THR:HG23	1.93	0.49
1:B:256:LEU:O	1:B:260:ARG:HB2	2.11	0.49
1:A:408:MSE:SE	1:A:692:HIS:HB2	2.63	0.49
1:B:807:LYS:HA	1:B:967:HIS:CD2	2.48	0.49
1:B:166:GLY:HA2	1:B:190:ILE:HG23	1.95	0.49
1:A:3:PHE:CE2	1:A:45:ARG:HG2	2.47	0.49
1:A:431:ARG:NE	1:A:632:PHE:O	2.42	0.49
1:B:170:ALA:HB3	1:B:932:ARG:HH22	1.78	0.49
1:B:69:MSE:SE	1:B:97:LEU:HD13	2.62	0.49
1:A:207:VAL:HG11	1:A:215:TRP:CD1	2.47	0.49
1:A:678:LYS:O	1:A:682:GLU:HG3	2.13	0.48
1:B:65:ASP:HB2	1:B:67:TRP:NE1	2.29	0.48
1:B:133:ARG:NH1	1:B:838:PRO:HB2	2.27	0.48
1:B:716:ILE:O	1:B:720:MSE:HG2	2.13	0.48
1:B:84:ILE:HA	1:B:95:VAL:O	2.12	0.48
1:B:221:ARG:HD3	1:B:772:GLU:HB3	1.94	0.48
1:A:122:ARG:HB2	1:A:125:ARG:HE	1.78	0.48
1:A:12:ASP:OD2	1:A:51:THR:OG1	2.32	0.48
1:A:39:GLU:OE2	1:A:41:ARG:NH2	2.46	0.48
1:A:805:LYS:HA	1:A:966:THR:O	2.14	0.48
1:A:218:GLU:OE2	1:A:222:ARG:NH2	2.47	0.48
1:A:311:LEU:HD23	1:A:327:ARG:HB3	1.96	0.48
1:A:377:ILE:HD12	1:A:406:MSE:HB3	1.96	0.48
1:B:354:ASP:O	1:B:358:MSE:HG2	2.14	0.48
1:A:585:PHE:CE1	1:A:643:TYR:HE1	2.32	0.48
1:A:866:ASN:OD1	1:A:867:ALA:N	2.47	0.48
1:B:441:PRO:HG2	1:B:444:TYR:CD2	2.49	0.48
1:B:584:PRO:HD3	1:B:593:ARG:CZ	2.44	0.48
1:B:415:ARG:NH2	1:B:935:GLU:OE2	2.47	0.47
1:B:866:ASN:OD1	1:B:867:ALA:N	2.47	0.47
1:B:133:ARG:NH2	1:B:956:ARG:HH22	2.12	0.47
1:B:324:HIS:HA	1:B:327:ARG:NH1	2.28	0.47
1:A:315:THR:HG21	1:A:321:MSE:HE1	1.97	0.47
1:A:781:HIS:CE1	1:A:783:LEU:HG	2.49	0.47
1:B:328:LEU:HB3	1:B:336:PHE:CZ	2.49	0.47
1:A:126:PHE:CE2	1:A:959:ALA:HB1	2.50	0.47
1:A:52:ARG:HG3	1:A:54:MSE:HG3	1.97	0.47
1:A:141:ARG:CZ	1:A:837:PRO:HD2	2.45	0.47
1:A:722:LEU:HD12	1:A:722:LEU:C	2.35	0.46
1:B:966:THR:OG1	1:B:968:GLN:OE1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:LEU:HD21	1:A:53:VAL:HG21	1.96	0.46
1:A:159:LEU:HD23	1:A:189:MSE:HE3	1.98	0.46
1:A:400:ARG:O	1:A:404:VAL:HG12	2.15	0.46
1:B:721:ASN:OD1	1:B:725:ILE:HD13	2.16	0.46
1:B:834:ARG:HH21	1:B:913:LYS:HZ1	1.60	0.46
1:B:859:GLU:O	1:B:863:ARG:HG3	2.16	0.46
1:A:13:THR:HG21	1:A:201:GLU:OE2	2.15	0.46
1:A:114:ARG:NH1	1:A:798:SER:OG	2.49	0.46
1:B:132:ALA:HB1	1:B:788:LEU:HD23	1.98	0.46
1:A:152:THR:O	1:A:765:ARG:NH1	2.46	0.46
1:B:434:HIS:N	1:B:608:ILE:O	2.49	0.46
1:A:846:ASP:OD1	1:A:849:GLY:N	2.48	0.46
1:A:934:ASP:OD2	1:B:37:THR:O	2.34	0.46
1:B:69:MSE:HG3	1:B:86:THR:C	2.35	0.46
1:B:96:ALA:O	1:B:97:LEU:HD12	2.16	0.46
1:B:370:LEU:HD13	1:B:386:LEU:HD21	1.97	0.46
1:A:28:ARG:HD2	1:A:241:ASP:OD2	2.16	0.46
1:A:69:MSE:SE	1:A:97:LEU:HB2	2.66	0.46
1:A:270:CYS:HB3	1:A:305:HIS:CG	2.51	0.46
1:B:586:ASN:HD21	1:B:589:LEU:HG	1.81	0.46
1:A:431:ARG:NH2	1:A:634:HIS:O	2.49	0.46
1:A:350:ARG:HB3	1:A:351:PRO:HD3	1.98	0.45
1:A:781:HIS:HE1	1:A:783:LEU:HG	1.80	0.45
1:A:596:ARG:NH2	2:A:1002:SO4:O2	2.44	0.45
1:B:535:HIS:H	1:B:538:MSE:SE	2.49	0.45
1:B:860:THR:HA	1:B:863:ARG:NE	2.31	0.45
1:B:809:LEU:O	1:B:967:HIS:NE2	2.48	0.45
1:B:924:LEU:O	1:B:928:ASN:N	2.46	0.45
1:A:149:GLY:HA2	1:A:778:THR:HG21	1.98	0.45
1:A:270:CYS:SG	1:A:302:LEU:HA	2.56	0.45
1:A:817:GLU:OE1	1:A:842:ARG:NH1	2.50	0.45
1:A:842:ARG:NH1	1:A:858:PHE:HA	2.30	0.45
1:B:404:VAL:HA	1:B:407:LEU:HD12	1.97	0.45
1:B:729:ASN:HB2	1:B:741:THR:OG1	2.16	0.45
1:B:9:TRP:HB2	1:B:32:LEU:HD21	1.98	0.45
1:B:485:TRP:CG	1:B:522:VAL:HG21	2.51	0.45
1:B:900:ARG:HH21	1:B:903:ILE:HG21	1.81	0.45
1:A:177:ASP:HB2	1:A:183:LYS:HG3	1.97	0.45
1:B:202:ARG:O	1:B:275:ASP:N	2.43	0.45
1:A:282:ALA:HB3	1:A:313:THR:HB	1.98	0.45
1:A:744:ASP:OD1	1:A:744:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:809:LEU:HB2	1:B:965:VAL:HG11	1.99	0.45
1:A:54:MSE:SE	1:A:81:LEU:HD11	2.67	0.45
1:A:342:PHE:O	1:A:346:GLN:HG2	2.17	0.45
1:A:861:PHE:O	1:A:865:LEU:HD13	2.16	0.45
1:B:564:GLU:OE2	1:B:593:ARG:CZ	2.65	0.45
1:A:742:PRO:HA	1:A:746:MSE:HE2	1.99	0.45
1:B:730:GLN:HB3	1:B:738:ILE:HG21	1.99	0.45
1:B:830:LEU:HB3	1:B:946:VAL:HG22	1.98	0.45
1:A:873:GLY:O	1:A:877:VAL:HG23	2.17	0.44
1:B:134:LYS:NZ	2:B:1003:SO4:O3	2.43	0.44
1:B:613:LEU:O	1:B:616:THR:HG22	2.15	0.44
1:A:474:TYR:CD2	1:A:484:TRP:HB3	2.52	0.44
1:B:569:GLY:HA3	2:B:1002:SO4:O4	2.18	0.44
1:A:737:MSE:HA	1:A:761:ILE:O	2.17	0.44
1:A:5:LEU:O	1:A:80:LEU:HD21	2.17	0.44
1:A:410:ARG:HG3	1:A:927:VAL:HG13	1.98	0.44
1:B:400:ARG:O	1:B:404:VAL:HG12	2.18	0.44
1:B:729:ASN:N	1:B:741:THR:O	2.49	0.44
1:A:540:ILE:HD12	1:A:540:ILE:HA	1.73	0.44
1:B:15:SER:C	1:B:18:GLY:H	2.19	0.44
1:B:311:LEU:HD23	1:B:327:ARG:HB3	1.99	0.44
1:B:842:ARG:NH1	1:B:858:PHE:HA	2.33	0.44
1:A:112:GLN:HG2	1:A:113:ASP:N	2.33	0.44
1:B:819:ILE:HB	1:B:959:ALA:HB3	1.99	0.44
1:B:842:ARG:NH1	1:B:858:PHE:CD1	2.83	0.44
1:A:274:TRP:O	1:A:307:PRO:HD2	2.18	0.44
1:A:464:ALA:O	1:A:468:LEU:HG	2.17	0.44
1:A:723:PHE:O	1:A:724:ASP:C	2.56	0.44
1:A:382:ILE:O	1:A:386:LEU:N	2.51	0.44
1:A:139:GLN:OE1	1:A:148:ARG:NH1	2.43	0.44
1:A:540:ILE:CD1	1:A:543:ARG:HH21	2.30	0.44
1:A:735:ASP:O	1:A:737:MSE:HG3	2.17	0.44
1:B:170:ALA:O	1:B:932:ARG:NH1	2.39	0.44
1:B:205:ILE:HG23	1:B:278:VAL:HB	1.99	0.44
1:A:415:ARG:HG2	1:A:415:ARG:NH1	2.33	0.43
1:A:269:LEU:HD23	1:A:269:LEU:HA	1.88	0.43
1:A:401:GLN:NE2	1:A:697:GLU:OE2	2.50	0.43
1:A:463:ARG:O	1:A:467:MSE:HG2	2.19	0.43
1:A:721:ASN:OD1	1:A:725:ILE:HD13	2.19	0.43
1:A:296:TYR:HE1	1:A:329:ARG:HH21	1.66	0.43
1:A:842:ARG:HH11	1:A:858:PHE:HD1	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:THR:C	1:B:934:ASP:OD2	2.57	0.43
1:A:139:GLN:HG3	1:A:779:TRP:CG	2.54	0.43
1:B:357:ALA:HB1	1:B:687:ARG:NH1	2.34	0.43
1:A:618:GLN:O	1:A:622:VAL:HG23	2.18	0.43
1:B:90:THR:OG1	1:B:92:GLU:HG3	2.17	0.43
1:B:846:ASP:OD1	1:B:850:ASN:N	2.34	0.43
1:A:277:LEU:HB2	1:A:306:VAL:HG11	2.01	0.43
1:A:578:MSE:HE1	1:A:594:ILE:HA	2.01	0.43
1:B:44:ALA:O	1:B:48:SER:HB3	2.17	0.43
1:B:105:LYS:HE2	1:B:105:LYS:HB2	1.87	0.43
1:B:805:LYS:HA	1:B:966:THR:O	2.19	0.43
1:A:37:THR:O	1:B:934:ASP:OD2	2.37	0.43
1:A:640:ARG:HA	1:A:643:TYR:HB3	2.00	0.43
1:B:589:LEU:HA	1:B:592:GLN:HB2	2.01	0.43
1:A:216:LEU:HD11	1:A:229:LEU:HD13	2.00	0.43
1:B:30:VAL:O	1:B:42:LEU:HD12	2.18	0.43
1:B:585:PHE:O	1:B:625:TYR:OH	2.37	0.43
1:A:5:LEU:HD12	1:A:22:VAL:HG12	2.01	0.43
1:A:258:PHE:HA	1:A:261:ARG:HH21	1.82	0.43
1:A:458:LYS:HD2	1:A:462:ASP:HB2	2.00	0.43
1:A:507:LEU:HD23	1:A:578:MSE:HE2	2.01	0.43
1:B:842:ARG:HH12	1:B:858:PHE:HD1	1.64	0.42
1:A:29:THR:HG21	1:A:241:ASP:HB3	2.01	0.42
1:B:350:ARG:HG3	1:B:354:ASP:OD2	2.18	0.42
1:B:646:VAL:HG12	1:B:650:LEU:HB2	2.00	0.42
1:A:370:LEU:HD13	1:A:386:LEU:CD2	2.49	0.42
1:B:410:ARG:HG3	1:B:927:VAL:CG1	2.47	0.42
1:B:562:CYS:SG	1:B:565:ILE:HD13	2.60	0.42
1:A:373:LEU:HD11	1:A:403:LEU:HD11	2.00	0.42
1:B:436:ILE:HG12	1:B:493:TRP:NE1	2.34	0.42
1:B:907:ARG:NH1	1:B:951:ASP:OD1	2.52	0.42
1:A:28:ARG:HB2	1:A:241:ASP:OD2	2.20	0.42
1:A:30:VAL:O	1:A:42:LEU:HD12	2.20	0.42
1:A:278:VAL:HG22	1:A:310:LEU:HD12	2.02	0.42
1:A:283:HIS:HB3	1:A:314:ALA:O	2.20	0.42
1:B:411:HIS:HD1	1:B:412:GLY:H	1.68	0.42
1:A:172:ARG:HH21	1:A:331:LEU:HA	1.85	0.42
1:B:110:LYS:HE2	1:B:113:ASP:OD2	2.20	0.42
1:B:356:VAL:O	1:B:360:LEU:HD12	2.20	0.42
1:A:431:ARG:NH1	1:A:591:GLU:OE2	2.53	0.42
1:A:722:LEU:HD12	1:A:722:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ARG:NH2	1:B:246:PHE:O	2.26	0.42
1:B:570:ARG:NH2	2:B:1002:SO4:O2	2.52	0.42
1:B:726:ILE:HG22	1:B:746:MSE:SE	2.70	0.42
1:A:122:ARG:HB2	1:A:125:ARG:HG3	2.02	0.42
1:A:122:ARG:HB3	1:A:124:ASP:OD1	2.20	0.42
1:A:548:ALA:HA	1:A:771:ARG:HD3	2.02	0.42
1:A:933:ASP:HB2	1:B:35:PRO:O	2.20	0.42
1:A:697:GLU:OE1	1:A:697:GLU:N	2.53	0.41
1:B:147:LEU:HD12	1:B:147:LEU:HA	1.88	0.41
1:B:185:ILE:HG22	1:B:189:MSE:SE	2.69	0.41
1:A:534:PHE:N	1:A:561:LEU:O	2.49	0.41
1:B:272:ALA:HB3	1:B:274:TRP:NE1	2.35	0.41
1:A:31:THR:OG1	1:A:42:LEU:HD13	2.21	0.41
1:A:538:MSE:HE3	1:A:538:MSE:HB3	1.71	0.41
1:A:889:GLN:O	1:A:892:GLU:HB3	2.20	0.41
1:A:309:VAL:CG1	1:A:311:LEU:CD1	2.98	0.41
1:A:349:TYR:CE1	1:A:688:LEU:HD12	2.52	0.41
1:A:382:ILE:HG22	1:A:386:LEU:HB2	2.02	0.41
1:A:121:ASP:N	1:A:799:SER:O	2.37	0.41
1:A:540:ILE:CG2	1:A:541:ILE:N	2.81	0.41
1:A:57:PRO:HA	1:A:71:VAL:HG12	2.01	0.41
1:A:256:LEU:HD12	1:A:259:ALA:HB3	2.01	0.41
1:B:17:LEU:O	1:B:36:SER:OG	2.30	0.41
1:B:263:LYS:O	1:B:267:GLU:N	2.49	0.41
1:B:489:PRO:HD2	1:B:613:LEU:HD21	2.02	0.41
1:B:744:ASP:N	1:B:744:ASP:OD1	2.53	0.41
1:A:875:LYS:HA	1:A:878:ASN:OD1	2.20	0.41
1:B:9:TRP:CZ2	1:B:52:ARG:HD3	2.56	0.41
1:B:189:MSE:HG3	1:B:223:PHE:CE1	2.56	0.41
1:A:306:VAL:HA	1:A:307:PRO:HD3	1.97	0.41
1:A:356:VAL:O	1:A:360:LEU:HD12	2.20	0.41
1:B:207:VAL:HG11	1:B:215:TRP:CD1	2.56	0.41
1:B:627:GLU:O	1:B:671:ARG:HD3	2.21	0.41
1:A:263:LYS:HZ1	1:A:301:GLN:HE22	1.68	0.41
1:A:299:ILE:O	1:A:303:ALA:N	2.30	0.41
1:A:319:LEU:HD23	1:A:323:SER:HB3	2.03	0.41
1:A:349:TYR:OH	1:A:686:ASP:OD1	2.29	0.41
1:A:805:LYS:HG2	1:A:966:THR:HG23	2.03	0.41
1:A:820:TYR:CE2	1:A:957:LEU:HD23	2.56	0.41
1:B:55:PHE:HD2	1:B:83:TYR:CZ	2.39	0.41
1:B:152:THR:O	1:B:765:ARG:NH1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:MSE:HE1	1:B:593:ARG:O	2.21	0.41
1:B:962:LEU:O	1:B:963:ILE:HD13	2.21	0.41
1:A:332:ASP:HB3	1:A:335:ARG:HB3	2.02	0.40
1:A:349:TYR:OH	1:A:688:LEU:HB2	2.20	0.40
1:A:381:ASP:OD1	1:A:381:ASP:N	2.52	0.40
1:A:207:VAL:HG12	1:A:211:LEU:HB2	2.04	0.40
1:B:505:LYS:HB3	1:B:550:PHE:CZ	2.56	0.40
1:B:586:ASN:ND2	1:B:589:LEU:HG	2.37	0.40
1:B:737:MSE:HE1	1:B:771:ARG:CZ	2.49	0.40
1:B:852:LEU:O	1:B:856:VAL:HG23	2.21	0.40
1:B:957:LEU:HD22	1:B:957:LEU:HA	1.97	0.40
1:B:483:THR:OG1	1:B:486:ASN:ND2	2.54	0.40
1:A:420:ASN:OD1	1:A:693:SER:HB3	2.21	0.40
1:A:615:LYS:HD3	1:A:615:LYS:HA	1.87	0.40
1:A:921:LEU:HA	1:A:921:LEU:HD23	1.83	0.40
1:A:287:TRP:HB3	1:A:326:ALA:HB1	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	965/968 (100%)	930 (96%)	35 (4%)	0	100	100
1	B	965/968 (100%)	928 (96%)	36 (4%)	1 (0%)	51	83
All	All	1930/1936 (100%)	1858 (96%)	71 (4%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	564	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	828/805 (103%)	810 (98%)	18 (2%)	52 79
1	B	828/805 (103%)	812 (98%)	16 (2%)	57 81
All	All	1656/1610 (103%)	1622 (98%)	34 (2%)	53 79

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	177	ASP
1	A	230	PHE
1	A	327	ARG
1	A	392	ASP
1	A	408	MSE
1	A	410	ARG
1	A	449	LYS
1	A	457	ARG
1	A	538	MSE
1	A	539	SER
1	A	554	ASP
1	A	619	SER
1	A	694	ASN
1	A	711	ASP
1	A	896	GLU
1	A	904	ASP
1	A	934	ASP
1	B	12	ASP
1	B	19	LEU
1	B	108	PHE
1	B	177	ASP
1	B	327	ARG
1	B	392	ASP
1	B	408	MSE
1	B	410	ARG
1	B	449	LYS

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Mol	Chain	Res	Type
1	B	457	ARG
1	B	538	MSE
1	B	539	SER
1	B	711	ASP
1	B	896	GLU
1	B	904	ASP
1	B	934	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	HIS
1	A	193	GLN
1	A	694	ASN
1	A	942	ASN
1	B	163	HIS
1	B	475	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	1001	-	4,4,4	0.14	0	6,6,6	0.18	0
2	SO4	B	1002	-	4,4,4	0.15	0	6,6,6	0.11	0
2	SO4	B	1001	-	4,4,4	0.14	0	6,6,6	0.13	0
2	SO4	A	1002	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	B	1004	-	4,4,4	0.15	0	6,6,6	0.04	0
2	SO4	A	1003	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	B	1003	-	4,4,4	0.14	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1002	SO4	2	0
2	B	1001	SO4	1	0
2	A	1002	SO4	1	0
2	A	1003	SO4	2	0
2	B	1003	SO4	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	944/968 (97%)	-0.03	12 (1%)	77	65	58, 105, 147, 170	0
1	B	944/968 (97%)	-0.05	9 (0%)	82	72	43, 99, 151, 199	0
All	All	1888/1936 (97%)	-0.04	21 (1%)	80	69	43, 102, 149, 199	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	49	PRO	5.4
1	A	813	THR	4.6
1	B	3	PHE	4.4
1	B	74	VAL	4.0
1	A	480	ASP	3.9
1	B	46	SER	3.7
1	A	27	ALA	3.6
1	A	74	VAL	3.5
1	B	870	ARG	3.3
1	B	24	ALA	3.1
1	A	17	LEU	3.0
1	B	48	SER	3.0
1	B	75	LYS	2.8
1	A	481	ASN	2.8
1	A	845	LEU	2.7
1	B	43	TYR	2.3
1	A	9	TRP	2.2
1	A	474	TYR	2.1
1	A	78	ASN	2.1
1	A	814	LEU	2.0
1	A	96	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	1003	5/5	0.90	0.18	113,118,134,134	0
2	SO4	A	1002	5/5	0.91	0.18	74,91,95,99	0
2	SO4	B	1002	5/5	0.94	0.21	74,75,82,103	0
2	SO4	A	1003	5/5	0.95	0.14	95,102,125,133	0
2	SO4	B	1004	5/5	0.97	0.21	84,98,114,122	0
2	SO4	B	1001	5/5	0.98	0.12	64,64,69,78	0
2	SO4	A	1001	5/5	0.99	0.17	56,57,70,88	0

6.5 Other polymers (i)

There are no such residues in this entry.